QUANTUM MECHANICS

Lecture schedule

- The course will consist of about 30 lectures and 5 tutorial sessions. The duration of each lecture and tutorial session will be 1.5 hours.
- We will meet thrice a week. The lectures are scheduled for 11:30 AM–1:00 PM on Tuesdays and Wednesdays, and during 9:00–10:30 AM on Fridays. We will be meeting in the discussion room in the top floor of the main building.
- The first lecture will be on August 6, 2008 and the last lecture will be on December 5, 2008.
- Changes in schedule, if any, will be notified sufficiently in advance.

Problem sheets, exams and grading

- The grading will be based on 3 problem sheets (each containing about 10 problems), a mid-semester and an end-of-semester exam.
- The 3 problem sheets, in total, will carry a 30% weight.
- The mid-semester exam will be on October 3, 2008. The exam will be for a duration of 1.5 hours and will carry a 30% weight.
- The end-of-semester exam will be on December 5, 2008. The exam will be of 3 hours duration and will carry a 40% weight.
- You will require a total of 50% to pass the course.

Syllabus and structure

1. **Introduction**
   (a) Limits of classical physics
   (b) Origins of quantum theory

2. **Wave aspects of matter**
   (a) Diffraction of matter waves
   (b) The double slit experiment with particles and waves
   (c) The Stern-Gerlach experiment
   (d) The superposition principle

Problem sheet 1

3. **The Schrodinger equation**
   (a) A brief digression on classical mechanics
   (b) The postulates of quantum mechanics – The Schrodinger equation
   (c) The probabilistic interpretation – The uncertainty principle
   (d) The classical limit – Ehrenfest's theorem

4. **Problems in one dimension**
   (a) The free particle
   (b) The infinite and finite square wells
   (c) Delta function potentials
   (d) The simple harmonic oscillator

Problem sheet 2

5. **Mathematical tools**
   (a) Vector spaces – Inner products – Matrices
   (b) Hilbert space – Observables – Hermitian operators – Eigen functions and eigen values
   (c) The generalized statistical interpretation
   (d) Non-commuting operators and the uncertainty relation
   (e) Dirac notation – The simple harmonic oscillator in the number basis

6. **The Schrodinger equation in three dimensions**
   (a) Central potentials – Infinite spherical well
   (b) The hydrogen atom
   (c) Algebra of angular momentum operators – Eigen values and eigen functions
   (d) Spin-$\frac{1}{2}$ systems – Larmor precession – Addition of angular momenta for spin-$\frac{1}{2}$ systems

Mid-semester exam

Problem sheet 3

7. **Symmetries**
   (a) Symmetries and conservation laws in classical mechanics
   (b) The Hamiltonian as the time evolution operator
   (c) Translation and rotation – Momentum and angular momentum operators as the generators of translation and rotation
   (d) Discrete symmetries – Parity – Time reversal

8. **Time-independent perturbation theory**
   (a) Non-degenerate and degenerate perturbation theory
   (b) The fine structure of hydrogen
   (c) Hyper-fine splitting

Problem sheet 4

9. **Time-dependent perturbation theory**
   (a) Two level systems – Sinusoidal perturbations and transition probabilities
   (b) Emission and absorption of radiation – Spontaneous emission
   (c) Quantization of the free electromagnetic field
   (d) Interaction of matter and radiation – Quantum dipole radiation

10. **Miscellany**
   (a) No cloning theorem
   (b) The EPR paradox – Bell's inequality
   (c) Bell states – Quantum teleportation
   (d) The Feynman-Kac formula – Propagators for the free particle and the harmonic oscillator
   (e) The WKB approximation – Tunneling – The connection formulas

End-of-semester exam

Essential texts

1. S. Gasiorowicz, *Quantum Physics*, Third edition (John Wiley and Sons, New York, 2003).
2. D. J. Griffiths, *Introduction to Quantum Mechanics*, Second edition (Pearson Education, Delhi, 2005).
3. W. Greiner, *Quantum Mechanics*, Fourth edition (Springer (India), Delhi, 2004).
4. R. Shankar, *Principles of Quantum Mechanics*, Second edition (Springer (India), Delhi, 2008).

Additional references

1. L. D. Landau and E. M. Lifshitz, *Quantum Mechanics* (Course of Theoretical Physics, Volume 3), Third Edition (Pergamon Press, New York, 1977).
2. J. .L. Powell and B. Crasemann, *Quantum Mechanics* (Narosa, Delhi, 1990).
3. J. J. Sakurai, *Modern Quantum Mechanics* (Addison-Wesley, Singapore, 1994).

Problem sheet 1

Origins of quantum theory and wave aspects of matter

1. (a) Consider a black body maintained at the temperature T. According to Planck's radiation law, the energy per unit volume within the frequency range $d\nu$ associated with the electromagnetic radiation emitted by the black body is given by

$$u_\nu \, d\nu = \left(\frac{8\,\pi\,h}{c^3}\right)\,\left(\frac{\nu^3}{\exp\left(h\,\nu/k_{\rm B}\,T\right)-1}\right)\,d\nu,$$

where h and $k_{\rm B}$ denote the Planck's and Boltzmann's constants, respectively.
The total energy emitted by the black body is then described by the integral

$$u = \int_0^\infty d\nu\, u_\nu.$$

Show that

$$u = \left(\frac{4\,\sigma}{c}\right)\,T^4, \quad \text{where} \quad \sigma = \left(\frac{\pi^2\,k_{\rm B}^4}{60\,\hbar^3\,c^2}\right) \quad \text{and} \quad \hbar = (h/2\pi).$$

(b) Obtain the Wien's law, viz. that $(\lambda_{\rm max}\,T) = b =$ constant, from Planck's radiation law.
Note: $\lambda_{\rm max}$ denotes the wavelength at which the energy density of radiation from the black body is the maximum.

(c) The experimentally determined values of the Stefan's constant σ and the Wien's constant b are given by

$$\sigma = 5.42\times10^{-6}\,{\rm J\,m^{-2}\,s^{-1}\,K^{-4}} \quad \text{and} \quad b = 2.9\times10^{-3}\,{\rm m\,K}.$$

Determine the values of the Planck's constant h and the Boltzmann's constant $k_{\rm B}$ from these values.

2. (a) Consider the emission of electrons due to photoelectric effect from a zinc plate. The work function of zinc is known to be 3.6 eV. What is the maximum energy of electrons ejected when ultra-violet light of wavelength 3000 Å is incident on the zinc plate?

(b) Recall that, in the Frank and Hertz experiment, the emission line from the mercury vapor was at the wavelength of 2536 Å. The spectrum of mercury has a strong second line at the wavelength of 1849 Å. What will be the voltage cooresponding to this line at which we can expect the current in the Frank and Hertz experiment to drop?

(c) Evaluate the numerical value of the Rydberg's constant $R_{\rm H}$ and compare with its experimental value of $109677.58\,{\rm cm}^{-1}$. How does the numerical value change if the finite mass of the nucleus is taken into account?

(d) Show that, in Compton scattering, the energy of the electron has a maximum in the forward direction and is given by

$$E = \left(\frac{h\,\nu_0}{1+(m_{\rm e}\,c^2/2\,h\,\nu_0)}\right),$$

where m_e denotes the mass of the electron and ν_0 is the mass of the incident photon.

3. Obtain the energy levels of the following systems using the Wilson-Sommerfeld quantization rule: (i) particle in a one-dimensional box, (ii) one-dimensional simple harmonic oscillator, and (iii) rigid rotator.

4. Consider a quantum mechanical particle propagating in the potential $V(x)$ and described by the wave function $\psi(x,t)$. The probability $P(x,t)$ of finding the particle at the position x and the time t is given by

$$P(x,t) = |\psi(x,t)|^2.$$

Using the one-dimensional Schrodinger equation, show that the probability $P(x,t)$ satisfies the conservation law

$$\left(\frac{\partial P(x,t)}{\partial t}\right) + \left(\frac{\partial j(x,t)}{\partial x}\right) = 0,$$

where the quantity $j(x,t)$ is the conserved current and is given by

$$j(x,t) = \left(\frac{\hbar}{2\,i\,m}\right)\left[\psi^*(x,t)\left(\frac{\partial\psi(x,t)}{\partial x}\right) - \psi(x,t)\left(\frac{\partial\psi^*(x,t)}{\partial x}\right)\right].$$

5. Given the time-independent wavefunction

$$\psi(x) = \left(\frac{\pi}{\alpha}\right)^{-1/4} e^{-(\alpha\,x^2/2)},$$

calculate the following quantities: (i) $\langle x\rangle$, (ii) $\langle x^2\rangle$, (iii) $\Delta x = \left[\langle x^2\rangle - \langle x\rangle^2\right]^{1/2}$, (iv) $\langle\hat{p}\rangle$, (v) $\langle\hat{p}^2\rangle$, (vi) $\Delta p = \left[\langle\hat{p}^2\rangle - \langle\hat{p}\rangle^2\right]^{1/2}$, and (vii) $(\Delta x\;\Delta p)$.

6. Establish the following operator relation:

$$\left[e^{(i\,\hat{p}\,a/\hbar)}\; x\; e^{-(i\,\hat{p}\,a/\hbar)}\right] \equiv (x+a).$$

Note: Given an operator $\hat{\mathcal{O}}$, the operator $e^{\hat{\mathcal{O}}}$ is defined as

$$e^{\hat{\mathcal{O}}} = \sum_{n=0}^{\infty}\left(\hat{\mathcal{O}}^n/n!\right).$$

This sheet has to be returned to Rajeev by noon on September 3, 2008.

Problem sheet 2

The Schrodinger equation in one dimension

1. (a) Recall that, we introduce the separation constant E to arrive at the time-independent Schrodinger equation from the time-dependent one. Show that, for normalizable solutions, the constant E must be *real*.

   (b) Prove that the time independent wave function $u_E(x)$ can always be taken to be real (unlike $\psi(x,t)$, which is necessarily complex).

   Note: This does not mean that every solution of the time-independent Schrodinger equation *is* real. If you have a solution that is not, then, what the above statement means is that, it can always be expressed as a linear combination of solutions (with the same energy) that *are* real.

   (c) Show that, if the potential $V(x)$ is an even function of x (i.e. $V(-x) = V(x)$), then $u_E(x)$ can always be taken to be either even or odd.

2. Consider a particle in the infinite square well. Let the initial wave function of the particle be given by
$$\psi(x,0) = A\,\left[u_1(x) + u_2(x)\right],$$
where $u_1(x)$ and $u_2(x)$ are the ground and the first excited states of the particle.

   (a) Normalize the wave function $\psi(x,0)$.

   (b) Obtain the wave function at a later time t, viz. $\psi(x,t)$, and show that the probability $|\psi(x,t)|^2$ is an oscillating function of time.

   (c) Evaluate the expectation value of the position in the state $\psi(x,t)$ and show that it oscillates. What are the angular frequency and the amplitude of the oscillation?

   (d) What will be the values that you will obtain if you measure the energy of the particle? What is the probability of obtaining these values?

   (e) Evaluate the expectation value of the Hamiltonian operator corresponding to the particle in the state $\psi(x,t)$. How does it compare with the energy eigen values of the ground and the first excited state?

3. Establish the completeness condition for the energy eigen states of a particle in an infinite square well.

4. Suppose that the Hamiltonian of a system depends on a parameter λ in some well-defined manner, $\hat{H} = \hat{H}(\lambda)$, with energy eigenvalues satisfying $\hat{H}(\lambda)\,u_E = E(\lambda)\,u_E$. (Remember that the eigenstates, u_E, will also depend on λ.)

   (a) Show that the dependence of the energy eigenvalue of a specific state on λ is then simply given by
$$\left(\frac{\partial E(\lambda)}{\partial \lambda}\right) = \left\langle \frac{\partial \hat{H}}{\partial \lambda}\right\rangle.$$
   Hint: Use the fact that probability is conserved.

   (b) Check this result explicitly for the infinite square well energy eigen states, using the mass m as the parameter.

5. Consider the following potential barrier:
$$V(x) = \left(\frac{V_0}{\cosh^2(\alpha\,x)}\right),$$
where $V_0 > 0$. Evaluate the tunneling probability for a particle scattering off the potential, assuming the energy of the particle to be less than V_0.

6. Obtain the normalized energy eigen functions of a particle moving in the potential $V(x) = (\alpha\, x)$, where $\alpha > 0$.

7. In this problem, we shall explore a few useful relations involving the Hermite polynomials.

   (a) According to the Rodrigues's formula

   $$H_n(x) = (-1)^n\, e^{x^2}\, \left(\frac{d}{dx}\right)^n \left[e^{-x^2}\right].$$

   Use this relation to obtain $H_3(x)$ and $H_4(x)$.

   (b) Utilize the following recursion relation

   $$H_{(n+1)}(x) = \left[2\, x\, H_n(x) - 2\, n\, H_{(n-1)}(x)\right],$$

   and the results of the above problem to obtain $H_5(x)$ and $H_6(x)$.

   (c) Using the expressions for $H_5(x)$ and $H_6(x)$ that you have obtained, check that the following relation is satisfied

   $$\left(\frac{dH_n}{dx}\right) = \left[2\, n\, H_{(n-1)}(x)\right].$$

   (d) Obtain H_0, $H_1(x)$ and $H_2(x)$ from the following generating function for the Hermite polynomials

   $$e^{-\left(z^2 - 2\, z\, x\right)} = \sum_{n=0}^{\infty} (z^n/n!)\;\; H_n(x).$$

8. Recall that the time-independent Schrodinger equation satisfied by the simple harmonic scillator of mass m and frequency ω is given by

   $$-\left(\frac{\hbar^2}{2\, m}\right)\left(\frac{d^2 u_E}{dx^2}\right) + \left(\frac{m}{2}\right)\, \omega^2\, x^2\, u_E = E\, u_E.$$

   In terms of the dimensionless variable

   $$\xi = (m\, \omega/\hbar)\; x,$$

   the above time-independent Schrodinger equation reduces to

   $$\left(\frac{d^2 u_E}{d\xi^2}\right) + \left(\mathcal{E} - \xi^2\right)\; u_E = 0,$$

   where $\mathcal{E}$ is the energy expressed in units of $(\hbar\, \omega/2)$, and is given by

   $$\mathcal{E} = (2\, E/\hbar\, \omega).$$

   According to the "wag-the-dog" method, one solves the above differential equation numerically, say, using Mathematica, varying $\mathcal{E}$ until a wave function that goes to zero at large ξ is obtained.

   Find the ground state energy and the energies of the first two excited states of the harmonic oscillator to five significant digits by the "wag-the-dog" method.

9. Find the first three allowed energies (to five significant digits) of the infinite square well, by wagging the dog.

10. Given a normalized wave function $\psi(x, t)$, the Wigner function $W(x, p, t)$ is defined as

   $$W(x, p, t) = \left(\frac{1}{\pi\, \hbar}\right) \int_{-\infty}^{\infty} dy\;\; \psi^*[(x + y), t]\;\; \psi[(x - y), t]\;\; e^{(2\, i\, p\, y/\hbar)}.$$

(a) Show that the the Wigner function $W(x,p,t)$ can also be expressed in terms of the momentum space wave function $\phi(p,t)$ as follows:

$$W(x,p,t) = \left(\frac{1}{\pi\,\hbar}\right) \int\limits_{-\infty}^{\infty} dq\ \ \phi^*[(p+q),t]\ \ \phi[(p-q),t]\ \ e^{-(2\,i\,q\,x/\hbar)}.$$

Note: Recall that, given the wave function $\psi(x,t)$, the momentum space wavefunction $\phi(p,t)$ is given by

$$\phi(p,t) = \left(\frac{1}{\sqrt{2\,\pi\,\hbar}}\right) \int\limits_{-\infty}^{\infty} dx\ \psi(x,t)\ e^{-(i\,p\,x/\hbar)}.$$

(b) Show that the Wigner function is a real quantity.

(c) Show that

$$\int\limits_{-\infty}^{\infty} dp\ \ W(x,p,t) = |\psi(x,t)|^2 \quad \text{and} \quad \int\limits_{-\infty}^{\infty} dx\ \ W(x,p,t) = |\phi(p,t)|^2.$$

(d) Consider the following normalized Gaussian wave packet

$$\psi(x,t) = \left(\sqrt{\pi}\,\alpha\,\mathcal{F}\,\hbar\right)^{-1/2}\ \ e^{i\,\left(\left[p_0\,(x-x_0)-(p_0^2\,t/2\,m)\right]/\hbar\right)}\ \ e^{-\left([x-x_0-(p_0\,t/m)]^2/2\,\alpha^2\,\hbar^2\,\mathcal{F}\right)},$$

where

$$\mathcal{F} = [1 + i\,(t/\tau)] \quad \text{and} \quad \tau = (m\,\hbar\,\alpha^2).$$

The peak of wave function is located at $x = [x_0 + (p_0\,t/m)]$, and the peak follows the trajectory of a classical free particle of mass m, whose position and momentum at the initial time $t = 0$ were x_0 and p_0, respectively.

i. Evaluate the Wigner function corresponding to this wave function.

ii. Plot the Wigner function, say, using Mathematica, at different times.

This sheet has to be returned to Rajeev by noon on September 26, 2008.

Mid-semester exam

1. Consider the one dimensional wave function

$$\psi(x) = A\ (x/x_0)^n\ \exp -(x/x_0),$$

where A, n and x_0 are constants. Determine the time-independent potential $V(x)$ and the eigen value E for which this wave function is an energy eigen function.

2. Consider a simple harmonic oscillator of mass m and angular frequency ω. The Hamiltonian operator of the oscillator can be written as

$$\hat{H} = \left(\hat{a}^\dagger\,\hat{a} + \frac{1}{2}\right)\ (\hbar\,\omega),$$

where $\hat{a}$ and $\hat{a}^\dagger$ are the annihilation and the creation operators, respectively. They are related to the position operator $\hat{x}$ and the momentum operator $\hat{p}$ by the following relations:

$$\hat{a} = \sqrt{\left(\frac{m\,\omega}{2\,\hbar}\right)}\ \left[\hat{x} + \left(\frac{i\,\hat{p}}{m\,\omega}\right)\right] \qquad \text{and} \qquad \hat{a}^\dagger = \sqrt{\left(\frac{m\,\omega}{2\,\hbar}\right)}\ \left[\hat{x} - \left(\frac{i\,\hat{p}}{m\,\omega}\right)\right],$$

In units such that $m = \hbar = \omega = 1$, let the un-normalized energy eigen function of a particular state be given by

$$\psi(x) = \left(2\,x^2 - 3\,x\right)\ \exp -(x^2/2).$$

Find that other two (un-normalized) eigen states that are closest in energy to the eigen state $\psi(x)$ above.

3. A free particle of mass m is constrained to move between two concentric impenetrable spheres of radii $r = a$ and $r = b$. Determine the ground state energy of the system and the normalized energy eigen function.

Note: This is a three dimensional problem.

4. Consider the description of the state of the electron in a basis where the operator $\hat{S}_z$ is diagonal. The basis spinors in such a case are given by

$$\chi_+ = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \qquad \text{and} \qquad \chi_- = \begin{pmatrix} 0 \\ 1 \end{pmatrix},$$

with the eigen values of the $\hat{S}_z$ operator in these states being $(\hbar/2)$ and $-(\hbar/2)$, respectively. Using the above basis construct the normalized eigen spinors of the operator $\hat{S}_y$ with eigen values $(\hbar/2)$ and $-(\hbar/2)$.

5. Let the dynamics of a particle moving in the one-dimensional potential $V(x)$ be governed by the Hamiltonian

$$H_0 = \left[(p^2/2m) + V(x)\right],$$

where $p = -\left[(i\hbar)\,(d/dx)\right]$ is the momentum operator. Let E_n^0, with $n = 1, 2, 3, \ldots$ be the discrete set of energy eigen values of the Hamiltonian H_0. Now, consider the new Hamiltonian

$$H = H_0 + (\lambda\,p/m),$$

where λ is a parameter. Given λ, m and E_n^0, find the eigen values of the Hamiltonian H.

$\boxed{\text{This test is for a duration of two hours.}}$

Problem sheet 3

Mathematical tools and the Schrodinger equation in three dimensions

Mathematical tools

1. (a) Suppose $\hat{\mathcal{O}}$ is a Hermitian operator and α is a complex number. Under what conditions (on α) is the operator $(\alpha\,\hat{\mathcal{O}})$ Hermitian.
   (b) When is the product of two Hermitian operators Hermitian?
   (c) Show that the position, momentum and the Hamiltonian operators are Hermitian.

2. A certain observable, say, $\hat{\mathcal{O}}$, has the following (3×3) matrix representation:

$$\hat{\mathcal{O}} = \left(\frac{1}{\sqrt{2}}\right) \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}.$$

   Determine the normalized eigen vectors of the observable and the corresponding eigen values.

3. Show that if two matrices commute in one basis, then they commute in any basis.

4. The coherent state $|\lambda\rangle$ of a one dimensional simple harmonic oscillator is defined to be the eigen state of the (non-Hermitian) annihilation operator $\hat{a}$ as follows:

$$\hat{a}\,|\lambda\rangle = \lambda\,|\lambda\rangle.$$

   (a) Show that

$$|\lambda\rangle = e^{-\left(|\lambda|^2/2\right)}\, e^{\left(\lambda\,\hat{a}^\dagger\right)}|0\rangle$$

   is a normalized coherent state.
   (b) Show that the state satisfies the minimum uncertainty relation.
   (c) The state $|\lambda\rangle$ can be expressed in terms of the n-th excited state $|n\rangle$ as

$$|\lambda\rangle = \sum_{n=0}^{\infty} f(n)\,|n\rangle.$$

   Show that the distribution of $|f(n)|^2$ with respect to n is of the Poisson form. Find the most probable value of n and, therefore, of E.

5. Let

$$\hat{J}_\pm = \left(\hat{a}_\pm^\dagger\,\hat{a}_\mp\right)\hbar, \qquad \hat{J}_z = \left(\hat{a}_+^\dagger\,\hat{a}_+ - \hat{a}_-^\dagger\,\hat{a}_-\right)(\hbar/2), \qquad \text{and} \qquad \hat{N} = \left(\hat{a}_+^\dagger\,\hat{a}_+ + \hat{a}_-^\dagger\,\hat{a}_-\right),$$

   where $\hat{a}_\pm$ and $\hat{a}_\pm^\dagger$ are the annihilation and the creation operators of two independent simple harmonic oscillators satisfying the usual commutation relations. Show that

$$[\hat{J}_z, \hat{J}_\pm] = \pm\,\hbar\,\hat{J}_\pm, \qquad [\hat{\mathbf{J}}^2, \hat{J}_z] = 0, \qquad \text{and} \qquad \hat{\mathbf{J}}^2 = \hat{N}\,\left[\left(\hat{N}/2\right) + 1\right]\left(\hbar^2/2\right).$$

   Note: This is known as Schwinger's model of angular momentum.

The Schrodinger equation in three dimensions

6. Consider the three dimensional 'particle in a box' wherein the potential is given by

$$V(\mathbf{x}) = \begin{cases} 0 & \text{when } 0 \le (x, y, z) \le a, \\ \infty & \text{otherwise.} \end{cases}$$

(a) Using the separation of variables in cartesian coordinates, solve the time-independent Schrodinger equation and obtain the stationary states and the corresponding energies.

(b) Let $E_1, E_2, E_3, \ldots$ denote the distinct energies in order of increasing energy. Determine E_1, E_2, E_3, E_4, E_5 and E_6, and their degeneracies.

(c) What is the degeneracy E_{14}, and why is this case interesting?

7. Using Mathematica, produce the plots described below for the wave functions describing the electron in a hydrogen atom.

   (a) The radial wave functions (as a function of the radius) for the following (n, l): $(1, 0)$, $(2, 0)$, $(2, 1)$, $(3, 0)$, $(3, 1)$ and $(3, 2)$.

   (b) Probability of the wave functions projected on to the (y, z)-plane for the following (n, l, m): $(2, 0, 0)$, $(3, 1, 0)$, $(4, 0, 0)$, $(4, 1, 0)$, $(4, 2, 0)$ and $(4, 3, 0)$.

   (c) Surfaces of constant probability for the following (n, l, m): $(2, 0, 0)$, $(2, 1, 0)$, $(2, 1, 1)$, $(3, 0, 0)$, $(3, 1, 0)$, $(3, 1, 1)$ $(3, 2, 0)$, $(3, 2, 1)$ and $(3, 2, 2)$.

   Note: These plots can be found, for instance, in D. J. Griffths, *Introduction to Quantum Mechanics*, Pearson Education, Singapore, 2005), see Figs. 4.4, 4.5 and 4.6.

8. (a) Prove that, for a particle that is moving in a potential $V(\mathbf{r})$, the rate of change of the expectation value of the orbital angular momentum operator $\hat{\mathbf{L}}$ is given by

   $$\left(\frac{d\,\langle\hat{\mathbf{L}}\rangle}{dt}\right) = \langle\hat{\mathbf{N}}\rangle,$$

   where $\mathbf{N} = -(\mathbf{r} \times \nabla V)$ is the torque.

   Note: This is the rotational analog of Ehrenfest's theorem.

   (b) Show that $(d\,\langle\hat{\mathbf{L}}\rangle/dt) = 0$ for any spherically symmetric potential.

   Note: This reflects the conservation of angular momentum in quantum mechanics.

9. Recall that the raising and lowering angular momentum operators, viz. $\hat{L}_{\pm}$, change the value of the magnetic quantum number m by one unit as follows:

   $$\hat{L}_{\pm}\,|l, m\rangle = A_{lm}\,|l, m\rangle,$$

   where A_{lm} is a constant. Assuming that $|l, m\rangle$ are normalized, determine A_{lm} using the algebra of the angular momentum operators.

10. Construct the spin matrices, viz. $\hat{S}_x$, $\hat{S}_y$, $\hat{S}_z$ and $\hat{\mathbf{S}}^2$, for a spin one particle.

This sheet has to be returned to Rajeev by noon on October 31, 2008.

Problem sheet 4

Time-independent perturbation theory

1. Show that, at the second order in time-independent, non-degenerate, perturbation theory, the state of the system is given by

$$\left|n^{(2)}\right\rangle = \sum_{k\neq n} \sum_{l\neq n} \left(\frac{V_{kl}\, V_{ln}\, \left|k^{(0)}\right\rangle}{\left(E_n^{(0)} - E_k^{(0)}\right)\left(E_n^{(0)} - E_l^{(0)}\right)}\right) - \sum_{k\neq n} \left(\frac{V_{nn}\, V_{kn}\, \left|k^{(0)}\right\rangle}{\left(E_n^{(0)} - E_k^{(0)}\right)^2}\right),$$

where $\left|k^{(0)}\right\rangle$ are the unperturbed states of the system, $E_k^{(0)}$ the corresponding eigen values, and

$$V_{nk} = \left\langle n^{(0)}\right| V \left|k^{(0)}\right\rangle,$$

with V being the perturbation.

2. (a) Show that, for an electron in the hydrogen atom,

$$\begin{aligned}\left\langle \frac{1}{r}\right\rangle &= \left(\frac{1}{n^2\, a}\right),\\ \left\langle \frac{1}{r^2}\right\rangle &= \left(\frac{1}{[l+(1/2)]\; n^3\, a^2}\right),\\ \left\langle \frac{1}{r^3}\right\rangle &= \left(\frac{1}{l\;[l+(1/2)]\;(l+1)\, n^3\, a^3}\right),\end{aligned}$$

where n and l are the principal and the azimuthal quantum numbers, and $a = \left(4\,\pi\,\epsilon_0\,\hbar^2/m_{\rm e}\,e^2\right)$ is the Bohr radius, with $m_{\rm e}$ denoting the mass of the electron, e the electronic charge, and ϵ_0 the permitivity of free space.

   (b) Use the above expressions to arrive at the following relativistic correction to the energy of the electron in the hydrogen atom:

$$E_{\rm r}^1 = -\left(\frac{(E_n)^2}{2\,m\,c^2}\right)\left[\left(\frac{4\,n}{l+(1/2)}\right) - 3\right],$$

and the following correction due to the spin-orbit coupling:

$$E_{\rm so}^1 = \left(\frac{(E_n)^2}{m\,c^2}\right)\left(\frac{n\;[j\,(j+1) - l\,(l+1) - (3/4)]}{l\;[l+(1/2)]\;(l+1)}\right),$$

where j is quantum number corresponding to the total angular momentum (i.e. orbital plus spin) of the electron. The quantity E_n in the above expressions is the Bohr energy associated with the level corresponding to the principal quantum number n, and is given by

$$E_n = -\left(\frac{m}{2\,\hbar^2}\right)\left(\frac{e^2}{4\,\pi\,\epsilon_0}\right)^2\left(\frac{1}{n^2}\right).$$

Note: $E_{\rm r}^1$ and $E_{\rm so}^1$ above have been evaluated at the first order in perturbation theory.

   (c) Also, show that, upon addition, $E_{\rm r}^1$ and $E_{\rm so}^1$ lead to the following expression for the fine-structure of hydrogen:

$$E_{\rm fs}^1 = \left(\frac{(E_n)^2}{2\,m\,c^2}\right)\left[3 - \left(\frac{4\,n}{j+(1/2)}\right)\right],$$

so that the energy E_n of the level n is modified to

$$E_{nj} = -\left(\frac{13.6\,{\rm eV}}{n^2}\right)\left[1 + \left(\frac{\alpha^2}{n^2}\right)\left(\frac{n}{j+(1/2)} - \frac{3}{4}\right)\right],$$

where $\alpha = (e^2/4\,\pi\,\epsilon_0\,\hbar\,c) \simeq (1/137.036)$ is the fine structure constant.

3. The exact fine structure formula for hydrogen (obtained from the Dirac equation without any recourse to perturbation theory) is given by

$$E_{nj} = \left(m_{\rm e}\, c^2\right) \left(\left[1 + \left(\frac{\alpha}{n - [j + (1/2)] + \sqrt{[j + (1/2]^2 - \alpha^2}}\right)^2\right]^{-1/2} - 1\right).$$

Expand this expression up to order α^4 (since $\alpha \ll 1$), and show that you recover the expression for E_{nj} in the previous problem.

4. Recall that the hyperfine structure of hydrogen is given by

$$E^1_{\rm hf} = \left(\frac{\mu_0\, g_{\rm p}\, e^2}{8\,\pi\, m_{\rm p}\, m_{\rm e}}\right) \left\langle\frac{3\,(\mathbf{S}_{\rm p}\cdot\hat{r})\,(\mathbf{S}_{\rm e}\cdot\hat{r}) - (\mathbf{S}_{\rm p}\cdot\mathbf{S}_{\rm e})}{r^3}\right\rangle + \left(\frac{\mu_0\, g_{\rm p}\, e^2}{3\, m_{\rm p}\, m_{\rm e}}\right) \langle\mathbf{S}_{\rm p}\cdot\mathbf{S}_{\rm e}\rangle\, |\psi(0)|^2,$$

where $m_{\rm p}$ denotes the mass of the proton, $g_{\rm p} = 5.59$ its gyromagnetic ratio, and μ_0 is the permeability of free space.

(a) Show that, when $l = 0$, the first term always vanishes.

(b) Show that, the ground state of hydrogen splits into a singlet and triplet state with the following energies:

$$E^1_{\rm hf} = \left(\frac{4\, g_{\rm p}\, \hbar^4}{3\, m_{\rm p}\, m_{\rm e}\, c^2\, a^4}\right) \begin{cases} +(1/4), \\ -(3/4). \end{cases}$$

(c) Also show that the gap between these two energy levels is

$$\Delta E = \left(\frac{4\, g_{\rm p}\, \hbar^4}{3\, m_{\rm p}\, m_{\rm e}\, c^2\, a^4}\right) = 5.88 \times 10^{-6}\,{\rm eV},$$

which corresponds to the wavelength of 21 cm.

5. Show that

$$\left[L^2, \left[L^2, \mathbf{r}\right]\right] = \left(2\,\hbar^2\right)\, \left(\mathbf{r}\, L^2 + L^2\, \mathbf{r}\right).$$

This sheet has to be returned to Sriram by noon on December 1, 2008.

End-of-semester exam

1. A particle of mass m is subjected to a force $\mathbf{F}(\mathbf{r}) = -\nabla_{\mathbf{r}} V(\mathbf{r})$ such that the wave function $\phi(\mathbf{p}, t)$ satisfies the following momentum space Schrodinger equation:

$$\left[\left(\mathbf{p}^2/2\,m\right) - a\,\nabla_{\mathbf{p}}^2\right]\,\phi(\mathbf{p}, t) = i\left(\frac{\partial \phi(\mathbf{p}, t)}{\partial t}\right),$$

where, for simplicity, we have set $\hbar = 1$, a is some real constant and

$$\nabla_{\mathbf{p}}^2 \equiv \left(\frac{\partial^2}{\partial p_x^2} + \frac{\partial^2}{\partial p_y^2} + \frac{\partial^2}{\partial p_z^2}\right).$$

Determine the force $F(\mathbf{r})$.

2. Consider a particle in the following square well:

$$V(x) = \begin{cases} 0, & \text{for} \quad |x| > a, \\ -V_0, & \text{for} \quad |x| \leq a. \end{cases}$$

What should be the value of $\left(V_0\, a^2\right)$, if there are to be four bound states?

3. Consider a particle that is *bound* in the central potential $V(r)$. Let the particle be in an eigen state, say, $|\psi_{E\ell m}\rangle$, of the energy (with eigen value E) and the angular momentum (with the azimuthal and the magnetic quantum numbers being ℓ and m, respectively). Evaluate the expectation value of the following operator in the state $|\psi_{E\ell m}\rangle$:

$$\hat{\mathbf{G}} = (\hat{\mathbf{r}} \cdot \hat{\mathbf{p}} + \hat{\mathbf{p}} \cdot \hat{\mathbf{r}})$$

4. Consider the following state with the azimuthal angular momentum $\ell = 1$:

$$|\psi\rangle = C_{-1}\,|1, -1\rangle + C_0\,|1, 0\rangle + C_1\,|1, 1\rangle.$$

Let $\hat{\mathbf{n}}$ be a unit vector along a certain direction. Construct the three states that are eigen states of the operator $(\hat{\mathbf{n}} \cdot \hat{\mathbf{L}})$ with the magnetic quantum numbers 0 and ± 1, In other words, express the coefficients C_{-1}, C_0 and C_1 for these three states in terms of the angles θ and ϕ that define the direction $\hat{\mathbf{n}}$.

5. Consider a charged particle that is exhibiting simple harmonic motion in one dimension. The particle is subjected to a constant electric field, say, in the positive direction along the axis of its motion. Calculate the shift in the energy of the nth excited state of the oscillator at the first and the second order in the magnitude of the electric field.

6. A charged particle is confined to a three dimensional cubical box of side $(2\,L)$. The particle is subjected to the following time-dependent electric field:

$$\mathbf{E} = \begin{cases} 0, & \text{for} \quad t < 0, \\ \mathbf{E}_0\, e^{-\alpha\, t}, & \text{for} \quad t > 0, \end{cases}$$

where α is a positive constant and the vector $\mathbf{E}_0$ is perpendicular to one of the faces of the box. Given that the charged particle is in the ground state at $t = 0$, calculate, to the lowest order in E_0, the probability that the particle is found in the first excited state as $t \to \infty$.

Additional problems

1. Show that the wave function

$$\psi(x,t) = \left(\frac{m\,\omega}{\pi\,\hbar}\right)^{1/2} \exp - \left[(m\,\omega/2\,\hbar)\ \left(x^2 + \left(a^2/2\right)\ \left(1 + e^{-2i\,\omega\,t}\right) + (i\,\hbar\,t/m) - 2\,a\,x\,e^{-i\,\omega\,t}\right)\right]$$

   satisfies the *time-dependent* Schrodinger equation for the simple harmonic oscillator of mass m and frequency ω.

   Note: The quantity a is a real constant with dimensions of length.

2. Evaluate $|\psi(x,t)|^2$, and describe the evolution of the wave packet.

3. Compute $\langle x \rangle$ and $\langle \hat{p} \rangle$, and show that the Ehrenfest's theorem is satisfied.